Ethylbenzene

100-41-4 | DTXSID3020596

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -42.1 °C

Global applicability domain: Inside

Local applicability domain index: 9.66e-01

Confidence level: 5.64e-01

Nearest Neighbors from the Training Set

Image not found
Ethylbenzene
Measured: -94.9
Predicted: -42.1

Image not found
ortho-Xylene
Measured: -25.2
Predicted: -35.2

Image not found
para-Xylene
Measured: 13.2
Predicted: -35.2

Image not found
m-Xylene
Measured: -47.8
Predicted: -35.2

Image not found
2,4,6-Trimethylstyrene
Measured: -37.0
Predicted: -37.0